Reconciliation of the Measurement of Parity-Nonconservation in Cs with the Standard Model

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Abstract

Contributions from the Breit interaction in atomic-structure calculations possibly explain the previously reported 2.5σ deviation from the Standard Model in the ^{133}Cs weak charge [S.C. Bennett and C.E. Wieman, Phys. Rev. Lett. **82**, 2484 (1999)]. The updated value of the weak charge is $Q_{\rm W}(^{133}{\rm Cs}) = -72.65(28)_{\rm expt}(34)_{\rm theor}$.

Atomic parity-nonconserving (PNC) experiments combined with accurate atomic structure calculations provide powerful constraints on "new physics" beyond the Standard Model of elementary particles [1]. Compared to high-energy experiments or low-energy scattering experiments, atomic single-isotope PNC measurements are uniquely sensitive to new isovector heavy physics [2]. Presently, the PNC effect in atoms has been most precisely measured by Wieman and co-workers using ^{133}Cs [3]. In 1999, Bennett and Wieman [4] updated the value of the Cs weak charge by measuring a supporting quantity, the vector transition polarizability β, and by re-evaluating the precision of atomic structure calculations [5,6] from the early 1990s. The determined weak charge [4] differed from the prediction [7] of the Standard Model by 2.5 standard deviations (σ). The value of the ^{133}Cs weak charge from Ref. [4] (together with other precision electroweak observables) has been employed in numerous articles. In particular, recent theoretical investigations [8,9] interpret this 2.5σ deviation as possible evidence for extra neutral vector Z-bosons.

The main focus of the two previous *ab initio* relativistic calculations for the atomic structure of ^{133}Cs [5,6] was the correlation contribution from the residual Coulomb interaction (i.e., beyond Dirac-Hartree-Fock level). In both calculations important chains of many-body diagrams were summed to all orders of perturbation theory. Here, these results will be referred to as "all-order Coulomb-correlated" values. The purpose of the present work is to evaluate rigorously contributions from the Breit interaction to PNC in ^{133}Cs. The previous calculations either omitted such contributions [6], or evaluated them only partially [5]. It is found that the Breit contribution corrects the derived weak charge by 0.9%, reducing the 2.5σ deviation from the Standard Model to 1.2σ. Including a correction for the neutron density distribution in the ^{133}Cs nucleus further reduces the deviation to 1.0σ. Thus the result reported here brings the most accurate atomic PNC measurement to date [3] into substantial agreement with the Standard Model.

The Breit interaction [10] arises due to an exchange of transverse photons between electrons. Its low-frequency limit is given by

$$B_{ij} = -\frac{1}{2r_{ij}}\left(\alpha_i \cdot \alpha_j + (\alpha_i \cdot \hat{r}_{ij})(\alpha_j \cdot \hat{r}_{ij})\right)$$

As emphasized by Lindroth *et al.* [11] small additional frequency-dependent contributions should be treated together with field-theoretical effects; such effects seem to be beyond the accuracy of modern atomic structure calculations for many-electron systems. It is convenient to separate the second-quantized Breit interaction into zero-, one-, and two-body parts normally ordered with respect to the core: $B = B^{(0)} + B^{(1)} + B^{(2)}$.

The parity-nonconserving amplitude for the $6S_{1/2} \to 7S_{1/2}$ transition in ^{133}Cs can be represented as a sum over intermediate states $mP_{1/2}$

$$E_{\rm PNC} = \sum_m \frac{\langle 7S|D|mP_{1/2}\rangle\langle mP_{1/2}|H_W|6S\rangle}{E_{6S} - E_{mP_{1/2}}} + \sum_m \frac{\langle 7S|H_W|mP_{1/2}\rangle\langle mP_{1/2}|D|6S\rangle}{E_{7S} - E_{mP_{1/2}}}\,. \tag{1}$$

Here D [12] and $H_{\rm W}$ are electric-dipole and weak interaction matrix elements, and E_i are atomic energy levels. It is convenient to break the total Breit correction $\delta E_{\rm PNC}$ into three distinct parts due to corrections in the weak interaction and dipole matrix elements, and energy denominators, respectively

$$\delta E_{\rm PNC} = E_{\rm PNC}(\delta H_{\rm W}) + E_{\rm PNC}(\delta D) + E_{\rm PNC}(\delta E)\,. \tag{2}$$

The overwhelming contribution from parity-violating interactions arises from the Hamiltonian

$$H_{\rm W} = \frac{G_F}{\sqrt{8}} Q_{\rm W} \rho_{\rm nuc}(r)\gamma_5\,, \tag{3}$$

where G_F is the Fermi constant, γ_5 is the Dirac matrix, and $\rho_{\rm nuc}(r)$ is the *neutron* density distribution. To be consistent with the previous calculations the $\rho_{\rm nuc}(r)$ is taken to be a *proton* Fermi distribution employed in Ref. [5]. The slight difference between the neutron and proton distributions will be addressed in the conclusion. The PNC amplitude is expressed in units of $10^{-11} i|e|a_0(-Q_{\rm W}/N)$, where $N = 78$ is the number of neutrons in the nucleus of ^{133}Cs. In these units the results of past calculations for ^{133}Cs are $E_{\rm PNC} = -0.905$, Ref. [5],

and $E_{\rm PNC} = -0.908$, Ref. [6]. The former value includes a partial Breit contribution $+0.002$, and the latter includes none. The reference many-body Coulomb-correlated amplitude

$$E^{C}_{\rm PNC} = -0.9075 \tag{4}$$

is determined as an average, with the partial Breit contribution removed from the value of Ref. [5].

Hartree-Fock analysis— Before proceeding to the correlated calculations discussed in the second part of this work, it is worth examining the Breit contribution to the PNC amplitude at the lowest-order level. The conventional Dirac-Hartree-Fock (DHF) equation reads

$$(h_{\rm D} + V_{\rm HF})\,\phi_i = \varepsilon_i \phi_i\,, \tag{5}$$

where h_D is the Dirac Hamiltonian including the interaction of an electron in state i with a finite-size nucleus. $V_{\rm HF}$ is a mean-field Hartree-Fock potential; this potential contains direct and exchange Coulomb interactions of electron i with core electrons. A set of DHF equations is solved self-consistently for core orbitals; valence wavefunctions and energies are determined subsequently by "freezing" the core orbitals. The Breit-Dirac-Hartree-Fock (BDHF) approximation constitutes the introduction of the one-body part of the Breit interaction $B^{(1)}$ into the above DHF equation

$$\left(h_{\rm D} + \tilde{V}_{\rm HF} + B^{(1)}\right)\tilde{\phi}_i = \tilde{\varepsilon}_i \tilde{\phi}_i\,. \tag{6}$$

Compared to the DHF equations, energies, wave-functions, and the Hartree-Fock potential are modified, as designated by tildes. This self-consistent BDHF approximation was used by Lindroth *et al.* [11] and a related iterative analysis was considered by Johnson *et al.* [13]. Both papers point out the importance of the "relaxation" effect, which leads to modification of the Hartree-Fock potential through adjustment of core orbitals. In the present work, the relaxation effect is taken into account automatically by direct integration of Eq. (6).

Most of the Breit contribution to the PNC amplitude can be determined by limiting the summation over intermediate states in Eq. (1) to the two lowest valence $P_{1/2}$ states: $6P_{1/2}$

and $7P_{1/2}$. In the DHF approximation one then finds $E_{\rm PNC} = -0.6888$ (90% of the total value). The lowest-order corrections to matrix elements and energy denominators calculated as differences between BDHF and DHF values are listed in Table I. The resultant BDHF corrections to $E_{\rm PNC}$ are:

$$\begin{aligned} E_{\rm PNC}(\delta H_{\rm W}) &= 0.0022\ (0.32\%)\,, \\ E_{\rm PNC}(\delta D) &= 0.0020\ (0.29\%)\,, \\ E_{\rm PNC}(\delta E) &= -0.0019\ (-0.28\%)\,. \end{aligned} \tag{7}$$

The sum of these three terms leads to $\delta E_{\rm PNC} = 0.0023$ in agreement with the 0.002 correction found by Blundell *et al.* [5,14]. Inclusion of intermediate states beyond $6P_{1/2}$ and $7P_{1/2}$ leads to a small additional modification to $\delta E_{\rm PNC}$ of -0.00004. Note that if experimental energies (which effectively include the Breit interaction) are used in the energy denominators of Eq. (1), then the $E_{\rm PNC}(\delta E)$ term must be excluded and the total correction becomes twice as large: $\delta E_{\rm PNC} = 0.0042$.

With further examination of the modifications of *individual* uncorrelated matrix elements presented in Table I, one notices the following.

(i) Weak interaction matrix elements are each reduced in absolute value by 0.3%, which is directly reflected in a 0.3% correction to the PNC amplitude.

(ii) Modification of dipole amplitudes is strongly nonuniform. There are substantial corrections only to the $6S_{1/2} - 7P_{1/2}$ (0.5%) and $7S_{1/2} - 6P_{1/2}$ (0.1%) matrix elements. The large 0.5% Breit correction to $\langle 6S_{1/2}|D|7P_{1/2}\rangle$ provides partial resolution to a long-standing 1.5% discrepancy of spectroscopic experiment [15] and *ab initio* calculations [16–18]. The relatively large Breit correction is caused both by an accidentally small matrix element and by admixture into $\langle 6S_{1/2}|D|7P_{1/2}\rangle$ from a 30 times larger $7S_{1/2} - 7P_{1/2}$ matrix element.

(iii) The largest modification in the energy denominators is 0.1% for $E_{7S} - E_{6P}$; however, this leads to a 0.3% correction $E_{\rm PNC}(\delta E)$. As recently emphasized by Dzuba *et al.* [19], such large sensitivity of the resulting PNC amplitude to small variations in individual atomic properties entering Eq. (1) arises due to a cancellation of relatively large terms in the sum

over states.

Correlated calculations— It is well known that correlations caused by residual Coulomb interactions not included in the Hartree-Fock equations can lead to substantial modifications of the lowest-order values. For example, the weak matrix element $\langle 6S_{1/2}|H_{\rm W}|6P_{1/2}\rangle$ is increased by a factor of 1.8 by correlations due to residual Coulomb interactions. It will be shown that the correlations are also important for a proper description of the Breit corrections.

The major correlation effects in atoms appear because of shielding of externally applied (e.g., electric) fields by core electrons and an additional attraction of the valence electron by an induced dipole moment of the core [20]. The former effect is described by contributions beginning at second order and the latter in third order of many-body perturbation theory (MBPT). Since these two effects lead to the dominant contributions in Coulomb-correlated calculations, the third-order analysis reported here seems sufficient [21].

MBPT calculations were performed with the two-body Breit interaction $B^{(2)}$ treated on equal footing with the residual Coulomb interaction. Sample many-body diagrams are presented in Fig. 1. To treat the one-body contribution $B^{(1)}$, an extension of the B-spline basis set technique [22] was developed, based on the Breit-Dirac-Hartree-Fock (BDHF) equation (6). Such a formulation made it possible to handle $B^{(1)}$ and the associated relaxation effect exactly. Contributions of negative-energy states, discussed for example in Ref. [23], were also included and found to be relatively small [24]. Two series of third-order calculations were performed, first with the Breit and Coulomb interactions fully included using the BDHF basis set, and second in the DHF basis set without the Breit interaction and negative-energy states. The obtained differences are the Breit corrections reported in Table I.

Breit corrections to ^{133}Cs hyperfine-structure magnetic-dipole constants A are discussed first, since these were considered in the literature previously. The correction to hyperfine constants is very sensitive to correlations: e.g., Ref. [17] found a numerically insignificant modification for A_{6S}, while Ref. [18,24] determined the modification to be large (-4.64 MHz),

and the approach reported here yields +4.89 MHz. In the calculation of Ref. [17] the correction was determined as a difference of the BDHF and DHF values, however such approach misses two-body Breit corrections of comparable size. In Ref. [18,24] a second order perturbation analysis was used for the Breit interaction, but the important relaxation effect discussed earlier was omitted. The present calculation incorporates all mentioned diagrams and is also extended to third order. Using this same calculational scheme, the corrections to hyperfine constants for other states of ^{133}Cs are +1.16 MHz for $7S_{1/2}$, -0.51 MHz for $6P_{1/2}$, and -0.146 MHz for $7P_{1/2}$. These corrections improve agreement with experiments for the *ab initio* all-order Coulomb-correlated calculations [17] to 0.1% for all states except $6P_{1/2}$ where the discrepancy becomes 0.5%.

Examination of the third-order corrections listed in Table I reveals the significant effect of correlations on the Breit contribution. For example, corrections to weak interaction matrix elements become three times larger than those in the lowest order. Compared to hyperfine-structure constants there is no strong cancellation of various MBPT contributions to the weak interaction matrix elements. Using third-order matrix elements and second-order energies the following *ab initio* corrections are determined: $E_{\rm PNC}(\delta H_{\rm W}) = 0.0043$, $E_{\rm PNC}(\delta D) = 0.0035$, and $E_{\rm PNC}(\delta E) = -0.0028$. Thus the lowest-order corrections given in Eq. (7) are amplified in higher orders. Discussion of modifications in individual matrix elements is similar to that presented above for the uncorrelated values.

To further improve the accuracy of the calculation, one can combine all-order Coulomb-correlated matrix elements and experimental energy denominators tabulated in Ref. [5] with the present third-order Breit corrections. The results are:

$$E_{\rm PNC}(\delta H_{\rm W}) = 0.0047\ (0.5\%)\,,$$
$$E_{\rm PNC}(\delta D) = 0.0037\ (0.4\%)\,. \qquad (8)$$

The Breit correction in energy-denominators $E_{\rm PNC}(\delta E)$ was set to zero because the experimental energies were extensively used in Ref. [6,5]. For example, the experimental energies were employed in eight out of ten test cases in the scatter analysis of Ref. [5]. The total 0.9%

Breit correction, $\delta E_{\rm PNC} = 0.0084$, is two times larger than the corresponding lowest-order modification, which is rather common in conventional Coulomb-correlated calculations. It is worth noting that an even larger 2% Breit correction was found in related calculations of the electric-dipole-moment (EDM) enhancement factor in thallium [11].

Discussion — Combining the calculated 0.9% Breit correction with the reference Coulomb-correlated value, Eq.(4), one obtains the parity-nonconserving amplitude

$$E_{\rm PNC}^{C+B}(^{133}{\rm Cs}) = -0.8991(36) \times 10^{-11} i(-Q_{\rm W}/N)\,.$$

A 0.4% theoretical uncertainty, mostly associated with higher-order Coulomb contributions, is assigned to the above result following the analysis of Ref. [4]. Since the Breit interaction contributes at the 0.9% level to the total PNC amplitude, even a conservative 10% uncertainty in $\delta E_{\rm PNC}$ barely affects the accuracy of $E_{\rm PNC}$. When $E_{\rm PNC}^{C+B}$ is combined with the experimental values of the transition polarizability β [4] and $E_{\rm PNC}/\beta$ [3], one obtains for the weak charge:

$$Q_{\rm W}(^{133}{\rm Cs}) = -72.65(28)_{\rm expt}(34)_{\rm theor}\,.$$

This value differs from the prediction [7] of the Standard Model $Q_{\rm W}^{\rm SM} = -73.20(13)$ by 1.2σ, versus 2.5σ of Ref. [4], where σ is calculated by taking experimental and theoretical uncertainties in quadrature. This 1.2σ deviation is slightly reduced further by taking into account corrections for the neutron nuclear distribution in ^{133}Cs, estimated but not included in the final $E_{\rm PNC}$ of Ref. [5]. Recently Pollock and Welliver [25] determined the relevant modification to be $\Delta Q_{\rm W}^{\rm SM} = +0.11$, which reduces the deviation from the Standard Model to 1.0 σ.

Is it possible to test the accuracy of the theoretical treatment of the Breit contribution for alkali-metal structure? One could consider the nonrelativistically forbidden magnetic-dipole transitions $nS_{1/2} - n'S_{1/2}$. A second-order analysis [23] demonstrated exceptionally large contributions from the Breit interaction and negative-energy states for such transitions; more accurate all-order calculations would be desirable. At the same time an accurate experimental value for the $7S - 6S$ transition in Cs is available [4].

The present calculation also provides a large Breit correction to the $6S_{1/2}-7P_{1/2}$ electric-dipole matrix element. Using the *ab initio* all-order Coulomb-correlated value from Blundell *et al.* [17], $\langle 6S_{1/2}||D||7P_{1/2}\rangle = 0.279$, and adding the 0.7% Breit correction of 0.0019, one finds $\langle 6S_{1/2}||D||7P_{1/2}\rangle = 0.281$ in much better agreement with the 0.284(2) experimental value of Shabanova *et al.* [15].

To summarize, third-order many-body calculations of the contribution of the Breit interaction to the ^{133}Cs parity-nonconserving amplitude $E_{\rm PNC}$ and relevant atomic properties are reported. The analysis reveals a 0.9% correction to $E_{\rm PNC}$ leading to a reduction to 1.2σ of the recently reported 2.5σ deviation [4] of the ^{133}Cs weak charge from the Standard Model value. If corrections for the neutron distribution in ^{133}Cs nucleus are included, then the agreement between the atomic PNC in ^{133}Cs and the Standard Model stands at 1.0σ. Thus the result reported here brings the most accurate atomic PNC measurement to date [3] into substantial agreement with the Standard Model.

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TABLES

TABLE I. Breit corrections to matrix elements and energy denominators in a.u.; $\delta X, \mathrm{I} \equiv \mathrm{X_{BDHF}} - \mathrm{X_{DHF}}$, and $\delta X, \mathrm{I} + \mathrm{II} + \mathrm{III}$ are the differences in the third order of MBPT.

	$6S_{1/2} - 6P_{1/2}$	$6S_{1/2} - 7P_{1/2}$	$7S_{1/2} - 6P_{1/2}$	$7S_{1/2} - 7P_{1/2}$
H_{W}, DHF	0.03159	0.01891	0.01656	0.009913
δH_{W}, I	-0.00010	-0.00006	-0.00005	-0.000031
δH_{W}, I+II+III	-0.00028	-0.00016	-0.00014	-0.000084
D, DHF	2.1546	0.15176	1.8017	4.4944
δD, I	0.0001	0.00073	0.0019	-0.0004
δD, I+II+III	-0.0004	0.00077	0.0020	-0.0012
ΔE, DHF	-0.041752	-0.085347	0.030429	-0.013166
$\delta \Delta E$, I	-0.000020	0.000003	-0.000030	-0.000007
$\delta \Delta E$, I+II	-0.000045	-0.000023	-0.000034	-0.000012

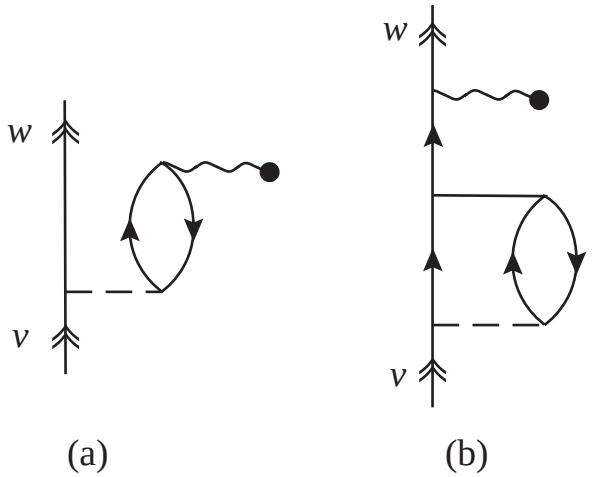

FIG. 1. Sample many-body diagrams included in the calculations. Dashed (solid) horizontal lines represent the Breit (Coulomb) interaction. All orbitals are obtained in the Breit-Dirac-Hartree-Fock approximation. Diagram (a) is one of the contributions in the random-phase approximation, and diagram (b) is one of the Brueckner-orbital contributions [20].

REFERENCES

[1] M.-A. Bouchiat and C. Bouchiat, Rep. Prog. Phys. **60** 1351 (1997); I.B. Khriplovich, *Parity Nonconservation in Atomic Phenomena* (Gordon & Breach, Philadelphia, 1991).

[2] M.J. Ramsey-Musolf, Phys. Rev. C **60**, 015501 (1999).

[3] C.S. Wood, S.C. Bennett, D. Cho, B. P. Masterson, J.L. Roberts, C.E. Tanner, and C.E. Wieman, Science **275**, 1759 (1997).

[4] S.C. Bennett and C.E. Wieman, Phys. Rev. Lett. **82**, 2484 (1999).

[5] S. A. Blundell, W.R. Johnson, and J. Sapirstein, Phys. Rev. Lett. **65**, 1411 (1990); Phys. Rev. D **45**, 1602 (1992).

[6] V.A. Dzuba, V.V. Flambaum, O.P. Sushkov, Phys. Lett. A **141**, 147 (1989).

[7] W.J. Marciano and J.L. Rosner, Phys. Rev. Lett. **65**, 2963 (1990); **68**, 898(E) (1992).

[8] J.L. Rosner, Phys. Rev. D, **61** 016006 (1999).

[9] R. Casalbuoni, S. De Curtis, D. Dominici, and R. Gatto, Phys. Lett. B **460**, 135 (1999).

[10] For a historical review of the Breit interaction see W.R. Johnson and K.T. Cheng in *Atomic Inner-Shell Physics*, ed. B. Crasemann (Plenum, New York, 1985), p. 1 and also Ref. [11]. Angular decomposition can be found in W.R. Johnson, S.A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 2764 (1988).

[11] E. Lindroth, A.-M. Mårtensson-Pendrill, A. Ynnerman, and P. Öster, J. Phys. B **22**, 2447 (1989).

[12] D are "stretched" amplitudes related to reduced matrix elements as $\langle nS_{1/2}|D|n'P_{1/2}\rangle = \langle nS_{1/2}||D||n'P_{1/2}\rangle/\sqrt{6}$.

[13] W.R. Johnson, S.A. Blundell, and J. Sapirstein, Phys. Rev. A **38**, 2699 (1988).

[14] The Breit correction in Ref. [5] also contains small random-phase-approximation di-

agrams in the Coulomb interaction for matrix elements of the weak interaction. The two-body Breit interaction has been disregarded in Ref. [5].

[15] L. Shabanova, Yu. Monakov, and A. Khlustalov, Opt. Spectrosk. **47**, 3 (1979) [Opt. Spectrosc. (USSR) **47**, 1 (1979)].

[16] V.A. Dzuba, V.V. Flambaum, and O.P. Sushkov, Phys. Lett. A **141**, 147 (1989).

[17] S.A. Blundell, W.R. Johnson, and J. Sapirstein, Phys. Rev. A **43**, 3407 (1991).

[18] M.S. Safronova, W.R. Johnson, A. Derevianko, Phys. Rev. A **60**, 4476 (1999).

[19] V.A. Dzuba, V.V. Flambaum, and O.P. Sushkov, Phys. Rev. A, **56**, R4357 (1997).

[20] W. R. Johnson, Z.W. Liu, and J. Sapirstein, At. Data Nucl. Data Tables, **64**, 279 (1996) and references therein.

[21] The random-phase-approximation sequence is limited to third order; and in addition only Brueckner-orbital corrections are included in the third order calculations.

[22] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 307 (1988).

[23] I. M. Savukov, A. Derevianko, H. G. Berry, and W.R. Johnson, Phys. Rev. Lett. **83**, 2914, (1999).

[24] A. Derevianko, E-print physics/0001046.

[25] S.J. Pollock and M.C. Welliver, Phys. Lett. B, **464**, 177 (1999).